

Optimizing photovoltaic performance of squaraine derivatives dyes: A DFT study on different anchoring groups

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Electronic Supplementary Information:

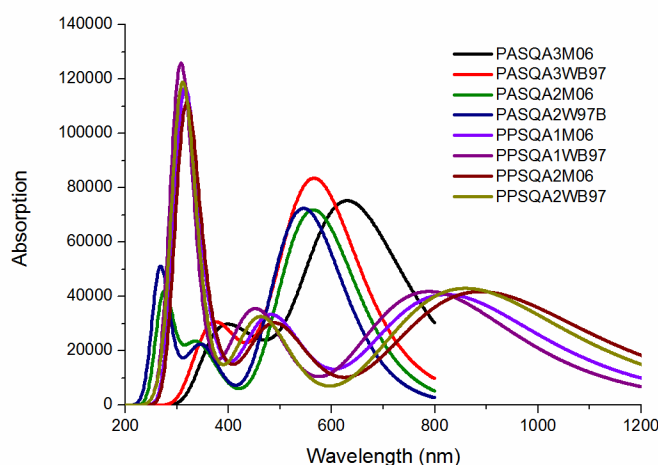
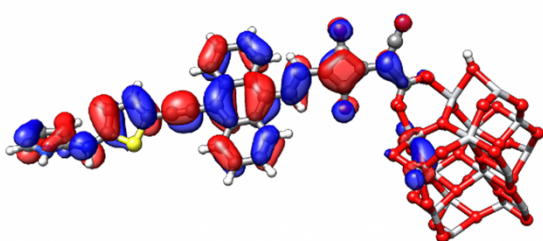
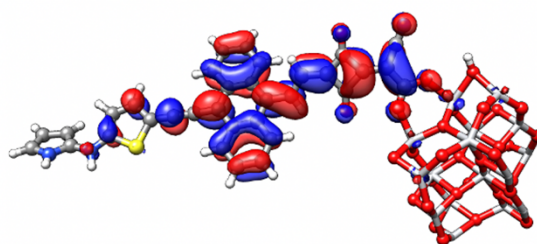


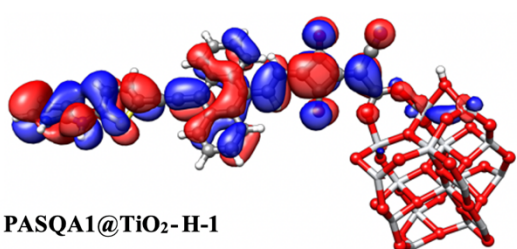
Figure S1: absorption spectra of dyes in acetonitrile at TD-M062X/6-311+G(2d,p)/SMD level and TD-wB97X-D/6-311+G(2d,p)/SMD level for most of the investigated dyes. The spectra are Gaussian broadened with 0.35 eV (half width half maximum).



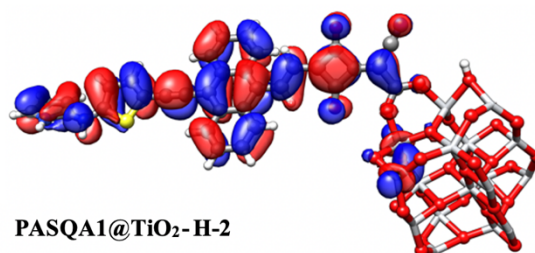
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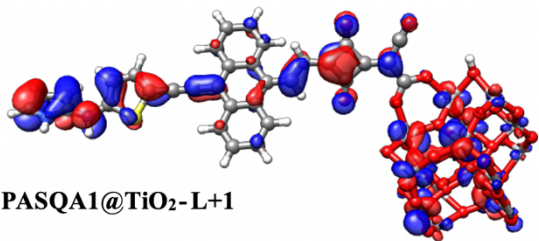
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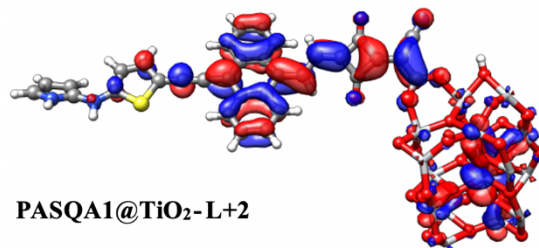
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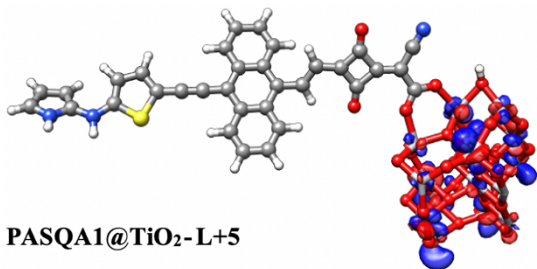
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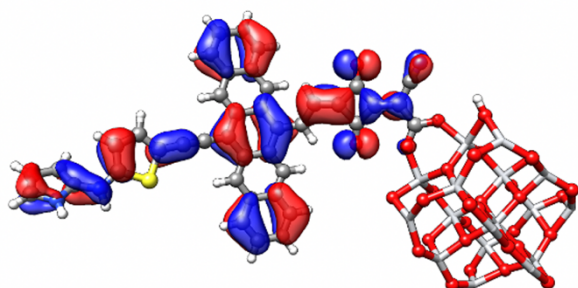
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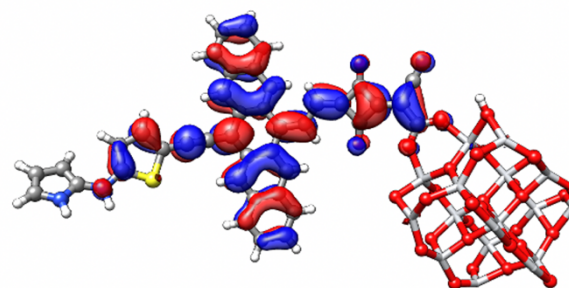
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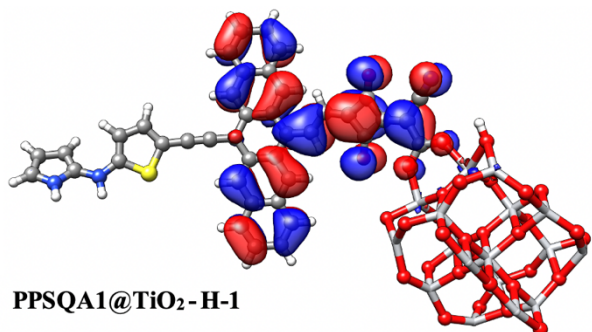
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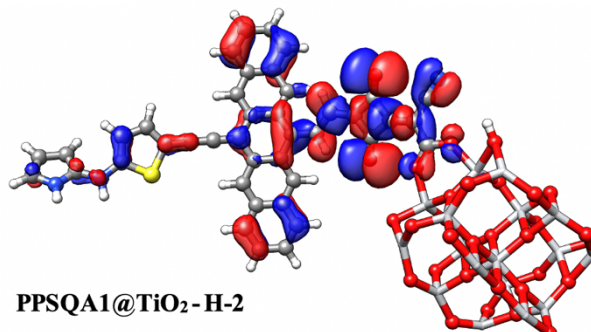
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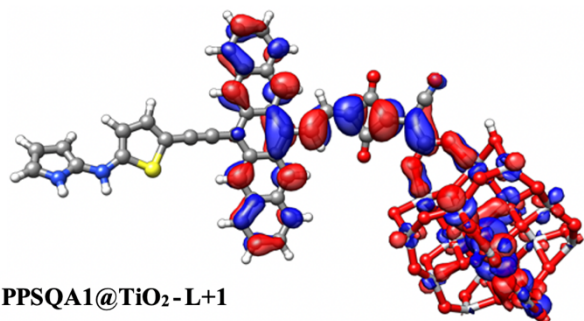
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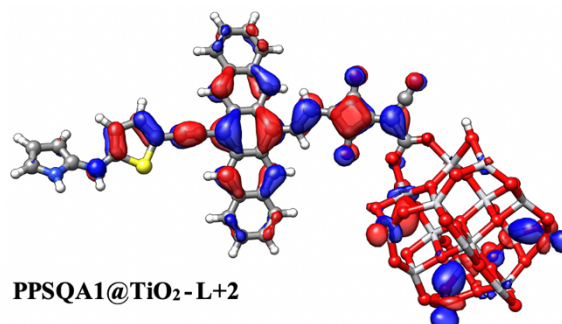
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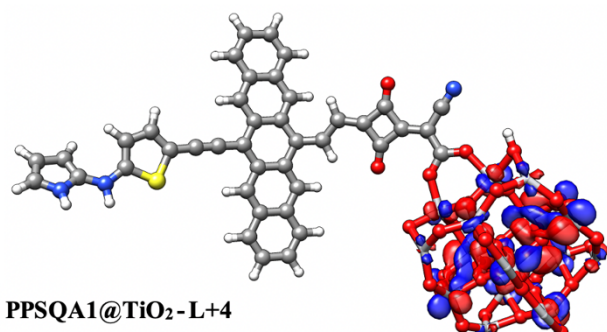
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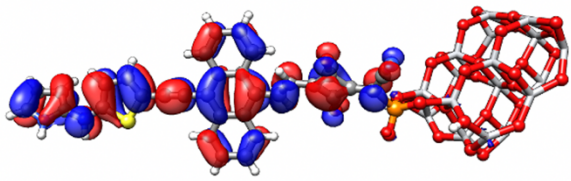
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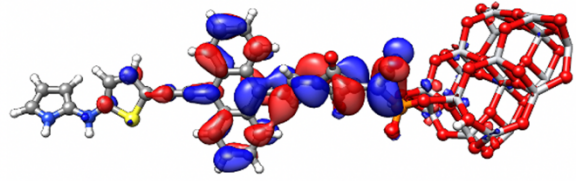
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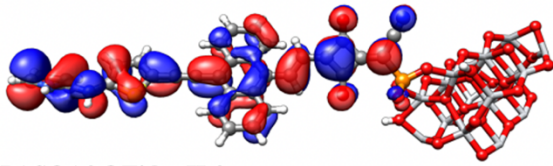
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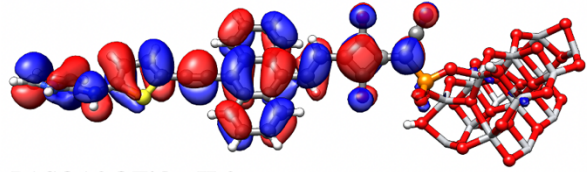
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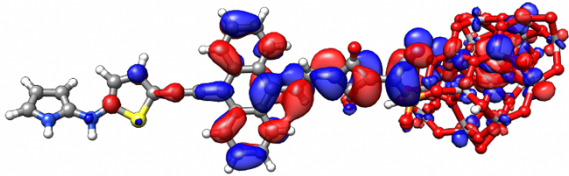
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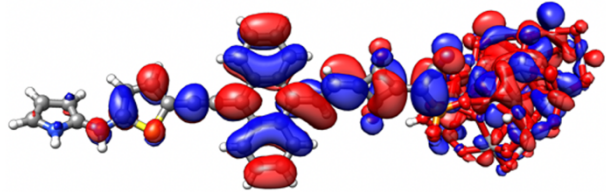
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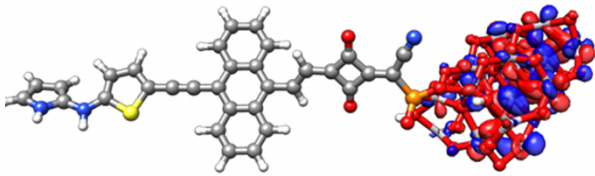
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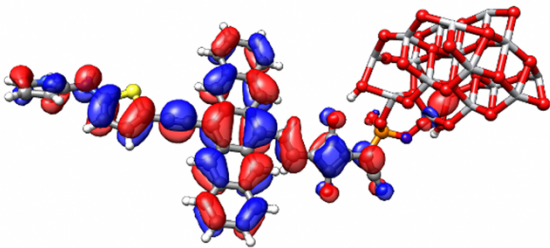
PASQA2@TiO₂ - L+1



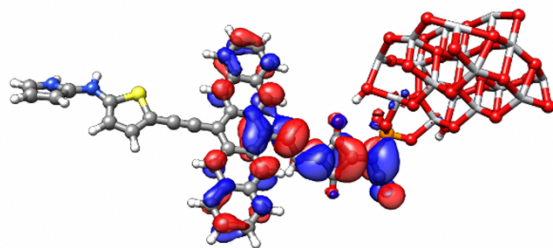
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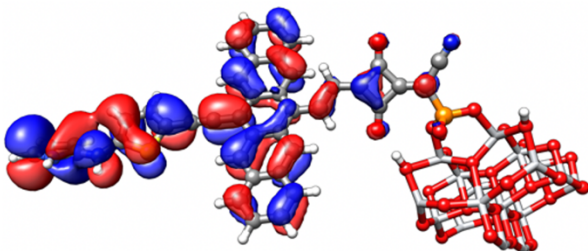
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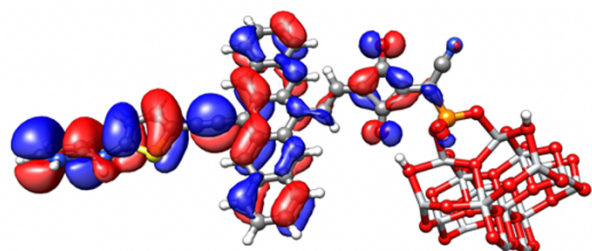
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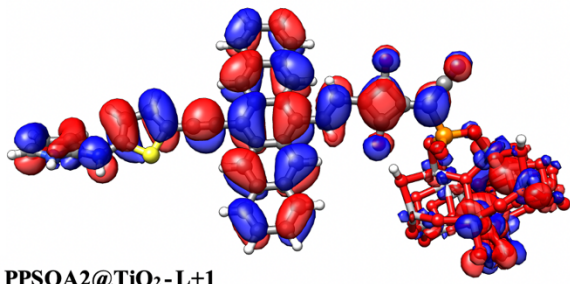
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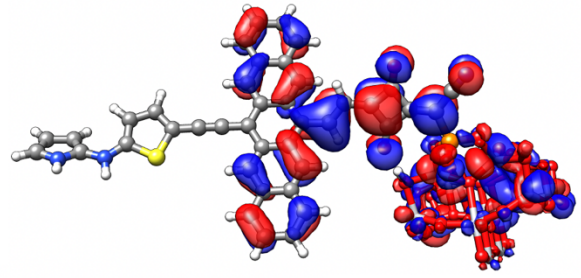
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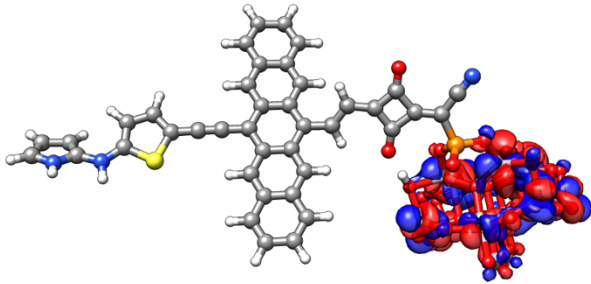
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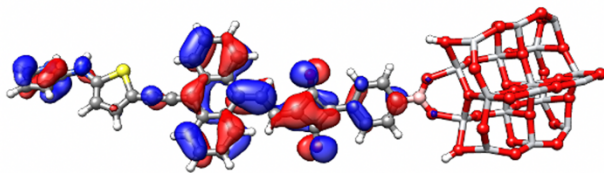
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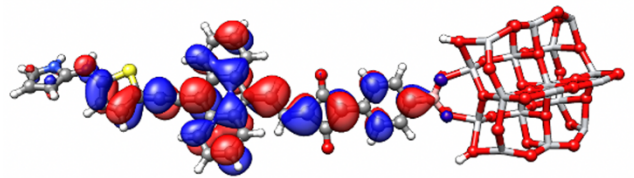
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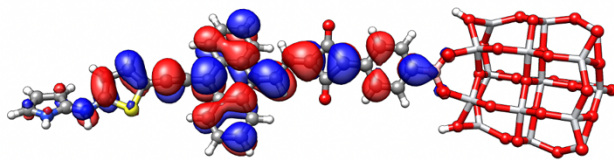
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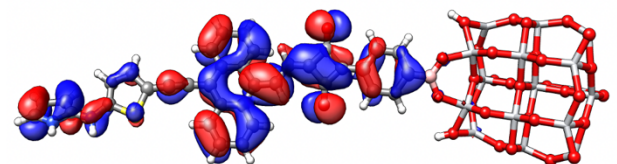
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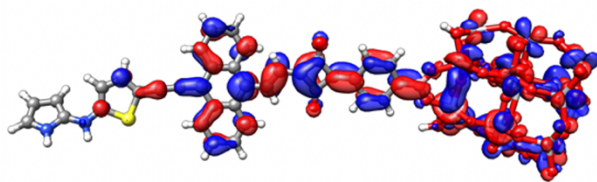
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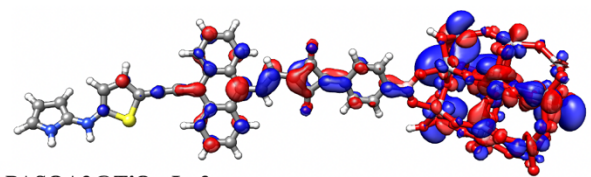
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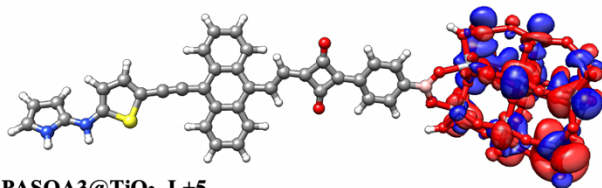
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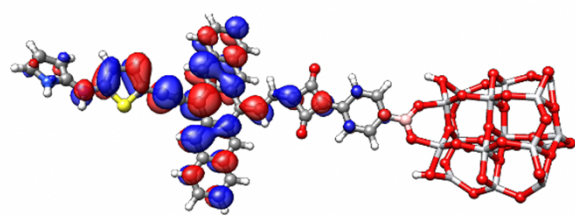
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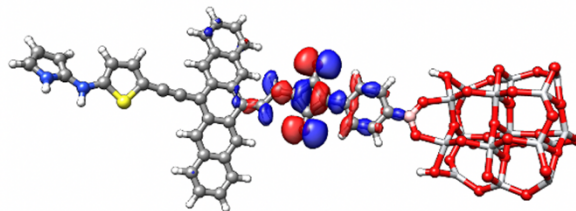
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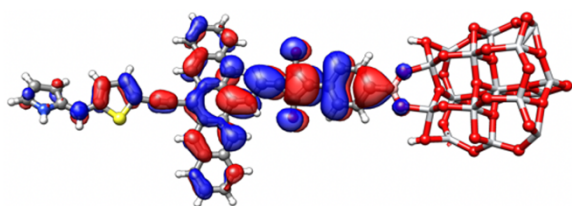
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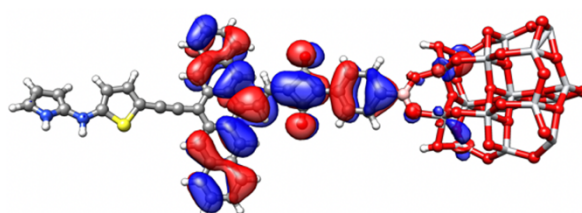
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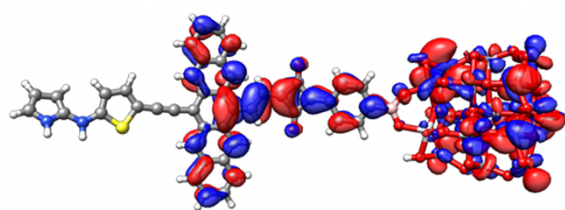
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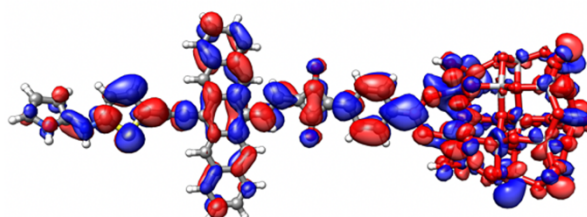
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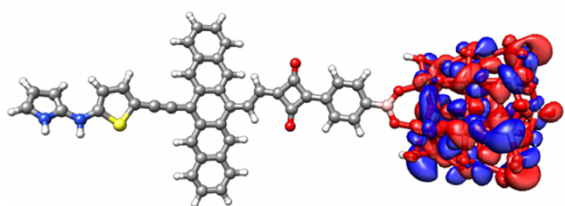
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PPSQA3@TiO₂ - L+1



PPSQA3@TiO₂ - L+3



PPSQA3@TiO₂ - L+5

Figure S2: Diagram of natural transition orbitals (NTO $S_0 \rightarrow S_1$) of the TiO₂@dyes in acetonitrile at TD-CAM-B3LYP/6-31G(d)/LANL2DZ level/SMD level. The surfaces are generated with an isovalue at 0.015.

Table S1: Absorption wavelengths, main contributions to the transitions, $S_0 \rightarrow S_1$ for the dyes in acetonitrile at TD-CAM-B3LYP/6-31G(d)/LANL2DZ/SMD level.

Compound	λ (nm)	Main contribution to the transition
PASQA1@TiO2	588.33	H→L (48%) H-1→L+2 (21%) H-2→L+1 ((19%) H→L+5 (8%)
PASQA2@TiO2	546.98	H→L (47%) H-3→L+1(27%) H-3→L+1 (17%) H→L+6 (7%)
PASQA3@TiO2	601.66	H→L (46%) H-2→L+1(23%) H-1→L+3(20%) H→L+5(6%)
PPSQA1@TiO2	1017.23	H→L (40%) H-1→L+2(29%) H-2→L+1 (22%) H→L+4 (6%)
PPSQA2@TiO2	910.15	H→L (42%) H-2→L+1 (25%) H-1→L+2(20%) H→L+4 (5%)
PPSQA3@TiO2	942.96	H→L(41%) H-1→L+3(30%) H-2→L+1(22%) H→L+5 (5%)

PSQA1

C	-3.10762900	0.71914200	-0.07602900
C	-5.68534700	0.27234900	0.00447200
O	-8.00493600	-0.09970700	-0.00228400
O	-6.68248000	-1.85852400	0.44810800
C	-6.78542200	-0.68122600	0.17119900
C	-0.92879800	-0.78268800	-0.04869500
H	-0.64395600	-1.83122300	-0.02724500
C	0.03925600	0.18910000	-0.05457900
O	-2.86934700	1.92866300	-0.11485600
O	-3.69053500	-2.53474400	-0.06943500
H	-8.67157000	-0.78890900	0.16195400
N	-6.34711700	2.75630900	-0.21256200
C	-6.03335000	1.64581600	-0.11482300
H	-0.29643500	1.22175900	-0.07947000
S	2.54639600	1.35452000	-0.05555500
C	3.94868400	0.31493000	0.04555800
C	3.57279900	-1.01981600	0.07480100
C	2.18158300	-1.19766800	0.04073500
C	1.44262600	-0.02936700	-0.02454300
N	5.19274900	0.87215100	0.08234700
H	4.27923500	-1.83278200	0.14035800
H	1.71552300	-2.17411100	0.07409900
H	5.25370400	1.87785300	0.17740000
N	7.52439800	0.76446500	0.55650500
C	8.61733800	-0.03798400	0.32730000
C	8.18685200	-1.13601500	-0.37694100
C	6.78512200	-0.99305000	-0.59638800

C	6.40977000	0.19818600	-0.00448100
H	7.53613200	1.63700100	1.06639500
H	9.59415000	0.24450200	0.68362100
H	8.80453100	-1.95627300	-0.70912500
H	6.14420600	-1.66735200	-1.13907000

PSQA2

C	-3.71268200	0.30446900	-0.08837900
C	-2.89611000	-0.91639700	-0.02169300
C	-1.67642800	-0.16789700	-0.02500700
C	-2.43574400	1.08204600	-0.10259900
C	-5.05244900	0.58217500	-0.11483600
C	-0.31284000	-0.52328400	0.02406500
H	-0.08002000	-1.58318700	0.07043200
C	0.69795600	0.39958200	0.01036100
O	-2.16197500	2.27453200	-0.15609200
O	-3.19486000	-2.13795400	0.01529200
N	-5.93508800	2.99305200	-0.25301200
C	-5.51170400	1.91569500	-0.19131600
H	0.41629400	1.44750600	-0.03573800
S	3.26422600	1.43475300	0.00094800
C	4.61044300	0.32265600	0.09848000
C	4.16509600	-0.98957000	0.13856800
C	2.76583900	-1.09372800	0.11482400
C	2.09010200	0.11098400	0.04678500
N	5.88394100	0.81098100	0.12184400
H	4.82870200	-1.83810600	0.20241800
H	2.24926400	-2.04415000	0.15465000
H	6.00173000	1.81214700	0.20835500
N	8.21954900	0.55287800	0.52277900
C	9.25585300	-0.30369900	0.23398800
C	8.74048800	-1.35098500	-0.49047100
C	7.34388200	-1.11938300	-0.66097200
C	7.05739000	0.07143400	-0.02085300
H	8.29751300	1.40451500	1.06115200
H	10.25797200	-0.09056700	0.56753400
H	9.29863900	-2.19407500	-0.86781100
H	6.64704600	-1.73650500	-1.20299800
P	-6.32594300	-0.70471200	-0.01707900
O	-7.55034200	-0.35451200	-0.77389500
O	-5.64118900	-2.05283900	-0.40809500
H	-4.61398100	-2.16641100	-0.19497500
O	-6.62119200	-0.92628700	1.56275400
H	-7.23854600	-0.26301600	1.91134200

PSQA3

C	2.47159800	0.76982300	0.01257200
C	1.75109200	-0.55008400	-0.03727300
C	0.47485000	0.13163500	-0.02597300
C	1.12618400	1.42398000	0.01962300
C	3.74362900	1.28807600	0.04686200
C	-0.86193100	-0.32841800	-0.04809800
H	-1.00783100	-1.40538200	-0.07848000
C	-1.94804300	0.50021500	-0.03243100
O	0.74817400	2.59615800	0.05072100
O	2.08920700	-1.73638600	-0.07221500
N	3.97694400	3.86047200	0.16127600
C	3.83902400	2.71235100	0.10825800
H	-1.76028000	1.56941100	-0.00024400
S	-4.59083000	1.31725200	-0.00650600

C	-5.85098000	0.10468100	-0.09396300
C	-5.30609600	-1.16497200	-0.12984500
C	-3.89644700	-1.16051500	-0.11114700
C	-3.31700100	0.08998200	-0.05357200
N	-7.15989500	0.50539900	-0.11503800
H	-5.89852600	-2.06499200	-0.18937000
H	-3.30909500	-2.06912200	-0.14871800
H	-7.34345100	1.49472300	-0.21674400
N	-9.48839300	0.14019500	-0.44184400
C	-10.46763700	-0.78750000	-0.16654800
C	-9.86977500	-1.84315000	0.47610100
C	-8.48036100	-1.54570200	0.60924800
C	-8.28167000	-0.30580700	0.03054500
H	-9.63284900	1.01571100	-0.92494500
H	-11.49131500	-0.61119500	-0.45267800
H	-10.36696800	-2.73605700	0.82306500
H	-7.73359000	-2.15451100	1.08996700
C	5.02652600	0.55626900	0.02970100
C	6.24985900	1.24927900	0.08007200
C	5.07899500	-0.84767700	-0.03987300
C	7.46052600	0.57149500	0.06150900
H	6.25772100	2.33094700	0.13465400
C	6.29592300	-1.51167800	-0.05785000
H	4.15720500	-1.41517600	-0.07845800
C	7.52134200	-0.82722400	-0.00868800
H	8.37929500	1.14578400	0.10188700
H	6.29448100	-2.59488200	-0.11230000
B	8.88684500	-1.58706500	-0.03130000
O	8.87038000	-2.95718900	-0.10589900
H	9.74119200	-3.37624300	-0.11549500
O	10.04416100	-0.85163800	0.02438500
H	10.85944500	-1.37010900	0.00637400

PASQA1

C	7.61758000	-0.08516400	-0.30277200
C	6.67375200	-1.06925200	-0.91761000
C	5.55238100	-0.39550200	-0.30496500
C	6.41727600	0.59551200	0.31144300
C	8.98400700	0.01470300	-0.36238500
C	4.15233800	-0.62951100	-0.31254200
H	3.80773300	-1.48327000	-0.88774300
C	3.26106300	0.17753200	0.32192500
O	6.22603900	1.57021200	1.02810900
O	6.82592600	-2.04730800	-1.64728800
H	3.67303600	1.05189700	0.81264100
S	-6.02496600	1.10831400	-0.16276200
C	-7.51530700	0.18478000	-0.21453300
C	-7.26735700	-1.16574400	-0.06118300
C	-5.89590500	-1.46208800	0.07323600
C	-5.06165500	-0.36599700	0.03677200
N	-8.69653600	0.84978300	-0.38651600
H	-8.04133700	-1.91729200	-0.06680200
H	-5.51347200	-2.46788900	0.18854900
H	-8.65096200	1.83746700	-0.60078500
N	-11.01425000	0.93428400	-0.92306500
C	-12.19156000	0.27457500	-0.65430800
C	-11.89480800	-0.78762900	0.16372400
C	-10.49028200	-0.76910600	0.41397300
C	-9.97813700	0.31398200	-0.27529400
H	-10.92198300	1.74730500	-1.51600600
H	-13.12459700	0.61972300	-1.06797600

H	-12.60255200	-1.50369300	0.55246700
H	-9.93771800	-1.45011400	1.03893100
C	-3.67185600	-0.30132500	0.12454500
C	-2.46063600	-0.22238500	0.19775600
C	-0.41670100	1.13319000	0.20075900
C	1.01637300	1.21745100	0.23018900
C	1.81053000	0.03932500	0.35211500
C	1.16095500	-1.21788700	0.51470600
C	-0.27333000	-1.30774100	0.44846100
C	-1.05391000	-0.13398100	0.27837700
C	-1.17831500	2.32956100	0.07218800
C	-0.57516700	3.55140800	-0.03126100
C	0.83706300	3.64114900	-0.02685200
C	1.60174800	2.51312100	0.08910500
C	1.87691600	-2.41822200	0.81139700
C	1.24395200	-3.62173300	0.95446400
C	-0.16125800	-3.71279600	0.81260900
C	-0.89368500	-2.58350500	0.57883200
H	-2.25820900	2.25736100	0.05661600
H	2.67733300	2.61347200	0.06613900
H	2.94565100	-2.37141500	0.95365900
H	-1.97162700	-2.64493400	0.50396300
H	-1.17424200	4.44951500	-0.12498100
H	1.31552900	4.60869800	-0.12413400
H	1.82017100	-4.50853900	1.19142900
H	-0.65503900	-4.67208000	0.91410500
C	9.71833400	-0.94863200	-1.11680500
N	10.34318100	-1.71432300	-1.71605600
C	9.83579400	1.02947100	0.27906900
O	11.04983400	1.05130900	0.17930700
O	9.15917300	1.94421300	0.99224900
H	9.81604900	2.55977600	1.36373000

PASQA2

C	6.97466600	0.31042300	0.44850900
C	6.01881400	1.32789600	0.99438000
C	4.91643000	0.64110400	0.33926400
C	5.81208900	-0.36053100	-0.21971100
C	8.32879200	0.13643800	0.55072900
C	3.51496600	0.86127000	0.31410100
H	3.14372300	1.67146300	0.93281200
C	2.66139300	0.04350900	-0.34744300
O	5.68370600	-1.34755900	-0.93987900
O	6.14699200	2.32103700	1.70531600
H	3.10803600	-0.85220200	-0.75006500
S	-6.49597100	-0.85711500	-0.24611700
C	-8.02126100	-0.09528300	0.17833000
C	-7.81508100	1.21488000	0.57419900
C	-6.46007800	1.59487700	0.55124100
C	-5.59372700	0.61233700	0.13975400
N	-9.14829900	-0.86499200	0.05694000
H	-8.59217600	1.88417600	0.88567700
H	-6.11553300	2.58010800	0.83565100
H	-8.98459000	-1.82575700	-0.20854500
N	-11.37977300	-1.60667000	0.07650300
C	-12.66814600	-1.17045200	0.25880100
C	-12.61375500	0.16350500	0.52931500
C	-11.24584300	0.56116200	0.51271900
C	-10.50226200	-0.56734100	0.22485500
H	-11.11606600	-2.55710300	-0.13678600
H	-13.50105200	-1.84878800	0.17978200

H	-13.45934700	0.80478800	0.72226800
H	-10.88752200	1.55485300	0.68468200
C	-4.21079900	0.66551900	0.00434200
C	-3.02074000	0.60968200	-0.14367400
C	-1.05585200	-0.83854500	-0.17279100
C	0.36954800	-1.00923000	-0.24276300
C	1.21844200	0.14596600	-0.41509900
C	0.60890500	1.40559400	-0.64324600
C	-0.80531400	1.57279800	-0.51833200
C	-1.62883400	0.45128300	-0.26294900
C	-1.89022100	-1.96764600	0.01998700
C	-1.37833000	-3.21664400	0.15145000
C	0.01706400	-3.40340400	0.11145500
C	0.85722100	-2.34170100	-0.06286300
C	1.36007500	2.51099500	-1.12959900
C	0.78843200	3.73295900	-1.32508300
C	-0.58701200	3.92453800	-1.06560600
C	-1.36057600	2.86569900	-0.69850900
H	-2.96110300	-1.81424100	0.06522200
H	1.91428100	-2.54522700	-0.05437300
H	2.39498900	2.36596900	-1.40643400
H	-2.42666000	2.99388200	-0.56360000
H	-2.03673100	-4.06318400	0.29844400
H	0.43321800	-4.39623600	0.23110100
H	1.38783700	4.55072300	-1.70584100
H	-1.03389500	4.90097000	-1.20446700
C	9.10638000	1.06636300	1.28527100
N	9.75582600	1.81098900	1.88857200
P	9.26943400	-1.21202200	-0.17499400
O	10.71347200	-1.21476300	0.15118700
O	8.48169600	-2.52340600	0.30886600
H	9.09104900	-3.27071800	0.43562500
O	8.97227700	-1.11539800	-1.75197800
H	9.78385400	-1.26200500	-2.26677700

PASQA3

C	6.38418500	0.30506000	0.24438800
C	5.52379500	1.46058400	0.43168900
C	4.36442400	0.71474600	-0.14042700
C	5.28138800	-0.45523200	-0.31807600
C	3.05738800	1.01618600	-0.38605000
H	2.72672400	2.01453600	-0.12176100
C	2.13532100	0.06958000	-0.90468500
O	5.13067700	-1.59622900	-0.76480200
O	5.65769200	2.60468100	0.87525200
H	2.54694000	-0.92819100	-0.98792400
S	-6.87726400	-1.22897300	0.17768700
C	-8.32903900	-0.38679000	0.69157500
C	-8.10098500	0.97133100	0.80419600
C	-6.77445500	1.33576100	0.50212700
C	-5.95201500	0.28504200	0.14474500
N	-9.46767500	-1.10924900	0.91389400
H	-8.85714500	1.67672300	1.11210500
H	-6.41166000	2.35417400	0.54846400
H	-9.39758100	-2.11765800	0.87577200
N	-11.66338300	-1.35637500	1.80446800
C	-12.86397100	-0.68772400	1.86809000
C	-12.70238600	0.51822200	1.23102200
C	-11.36081400	0.58327000	0.75077300
C	-10.74724000	-0.59781700	1.12355500
H	-11.47816500	-2.26334600	2.20954900

H	-13.71635300	-1.12904100	2.35754600
H	-13.46072700	1.27669000	1.11093500
H	-10.91581000	1.38430300	0.18482200
C	-4.60790800	0.28894900	-0.20615300
C	-3.42825400	0.27460300	-0.52229500
C	-1.42380800	-0.97098400	-1.21477200
C	-0.01418900	-1.00038200	-1.42845100
C	0.78356400	0.20570400	-1.20116900
C	0.06430900	1.47406700	-1.21486900
C	-1.34351100	1.49745000	-0.98007100
C	-2.07675100	0.26476600	-0.87264700
C	-2.16503700	-2.17060200	-1.35209800
C	-1.56210500	-3.34937100	-1.72307500
C	-0.18110100	-3.37261200	-1.97708000
C	0.56763900	-2.22461700	-1.82558500
C	0.70531400	2.70044700	-1.49345700
C	0.02921300	3.90349900	-1.45179500
C	-1.33427800	3.92891600	-1.12204400
C	-2.00462500	2.74704100	-0.90337100
H	-3.23309300	-2.14549300	-1.17587200
H	1.62660600	-2.26870400	-2.04156700
H	1.74450900	2.69880700	-1.78752400
H	-3.06749000	2.76269200	-0.69774400
C	7.76553900	0.02616600	0.50743100
C	8.32666300	-1.23561400	0.20985000
C	8.61335000	1.00503500	1.07187900
C	9.66295300	-1.49512100	0.46551400
H	7.69511600	-2.00180400	-0.22322500
C	9.94756500	0.72898800	1.32050300
H	8.20454000	1.97986700	1.30875900
C	10.51265800	-0.52483200	1.02619500
H	10.06250800	-2.47424600	0.22480400
H	10.57127600	1.50316400	1.75397000
B	12.01812800	-0.82552900	1.30794500
O	12.79568600	0.17097300	1.84500800
H	13.71904200	-0.06984000	1.99771600
O	12.50507300	-2.07393700	1.00695300
H	13.44330700	-2.20286100	1.19928800
H	0.55132900	4.82374800	-1.68619600
H	-1.86638800	4.87182200	-1.07211400
H	0.29847600	-4.28968000	-2.29876200
H	-2.15275600	-4.25129900	-1.83376200

PPSQA1

C	-7.56298200	0.01621600	0.41559300
C	-6.64666300	-0.99928300	1.01593500
C	-5.51108400	-0.37547600	0.37225300
C	-6.35582100	0.63903700	-0.23904600
C	-8.92140300	0.19071200	0.52910100
C	-4.12321400	-0.64953000	0.36899800
H	-3.79819900	-1.50417800	0.95313100
C	-3.21468800	0.13873900	-0.27731600
O	-6.14256300	1.59956500	-0.96940200
O	-6.81792400	-1.96708100	1.75562300
H	-3.62507300	1.01724300	-0.76077200
S	6.05739600	1.09250500	0.18973500
C	7.54929100	0.18158800	0.33101300
C	7.30671700	-1.17942800	0.28616700
C	5.93997300	-1.49106500	0.16322700
C	5.10031400	-0.39749600	0.10159700
N	8.72702700	0.85976700	0.45820800

H	8.08375900	-1.92416600	0.36107500
H	5.56150400	-2.50418500	0.12648300
H	8.67882800	1.86067300	0.59914500
N	11.04344300	0.97975200	0.99748300
C	12.22200500	0.30746200	0.77149700
C	11.92947400	-0.80158200	0.01597700
C	10.52619500	-0.79999100	-0.23918000
C	10.01044900	0.32075400	0.38396000
H	10.94806200	1.82647700	1.54081800
H	13.15333900	0.67767500	1.16692400
H	12.63959000	-1.53776300	-0.32820900
H	9.97598700	-1.51724100	-0.82458400
C	3.71474700	-0.34603800	-0.00799600
C	2.50308800	-0.27405000	-0.10542000
C	0.47421000	1.08816100	-0.28085100
C	-0.97184300	1.17998600	-0.31935700
C	-1.77595300	-0.00772200	-0.32227300
C	-1.12739100	-1.28271000	-0.37546500
C	0.31767200	-1.37528700	-0.27805500
C	1.10457000	-0.18895500	-0.21594400
C	1.24101000	2.26687300	-0.28075500
C	0.66440800	3.52802100	-0.30633900
C	-0.77345900	3.63046800	-0.31268800
C	-1.53891300	2.47117400	-0.30567900
C	-1.83731700	-2.48202000	-0.58548600
C	-1.22307300	-3.72765600	-0.61198700
C	0.20330000	-3.81581800	-0.42260200
C	0.92845000	-2.64210600	-0.27762700
H	2.32091700	2.18911700	-0.25820900
H	-2.61253800	2.59158500	-0.28425800
H	-2.90187800	-2.44636800	-0.76131900
H	2.00556200	-2.70424200	-0.18430500
C	-9.66908000	-0.69274700	1.36234600
N	-10.30596300	-1.38726500	2.03222500
C	-9.74750800	1.22045900	-0.11830100
O	-10.94682900	1.33887200	0.06510200
O	-9.06851300	2.03117400	-0.94707700
H	-9.70854400	2.67003800	-1.30821900
C	-1.36716300	4.93302200	-0.32005800
C	-0.58964100	6.05270000	-0.32645500
C	0.83555700	5.94976500	-0.32365600
C	1.44221800	4.72921400	-0.31323100
C	0.82134100	-5.10647600	-0.43106900
C	0.07726600	-6.23195300	-0.62562000
C	-1.33434700	-6.14443600	-0.82885100
C	-1.96253000	-4.93454500	-0.82525000
H	-2.44896800	5.00970600	-0.32262900
H	-1.04881100	7.03445100	-0.33363800
H	1.43148600	6.85502100	-0.32874100
H	2.52357300	4.64683500	-0.30892100
H	1.89380700	-5.16927000	-0.28270100
H	0.55301000	-7.20578000	-0.63084300
H	-1.90347200	-7.05341200	-0.98554000
H	-3.03427300	-4.86619900	-0.97645900

PPSQA2

C	7.00997100	-0.58984500	-0.11647600
C	6.03495400	-1.69490300	-0.33546200
C	4.93104200	-0.78098000	-0.12052800
C	5.85158200	0.32030700	0.09728700
C	8.36679800	-0.53315300	-0.10256800

C	3.53515900	-0.90605500	-0.22827600
H	3.15608300	-1.85512100	-0.60356700
C	2.70143600	0.12945800	0.07248300
O	5.73392700	1.51315300	0.35186100
O	6.13652500	-2.88374600	-0.59135400
H	3.19705500	1.05917700	0.30934100
S	-6.70903200	1.02603100	0.49468600
C	-8.12445200	0.10881700	0.01172300
C	-7.77949800	-1.03630900	-0.63870100
C	-6.39168500	-1.19741200	-0.75723900
C	-5.64378700	-0.18440600	-0.20676400
N	-9.34196400	0.59777900	0.31103600
H	-8.49662200	-1.74935000	-1.03004400
H	-5.93731800	-2.04849300	-1.24085200
H	-9.37490900	1.49747900	0.76387700
N	-11.68673900	0.71356000	0.43984700
C	-12.79909600	-0.02810700	0.14517900
C	-12.37219700	-1.21158500	-0.41010000
C	-10.94879200	-1.18837900	-0.45273600
C	-10.56551500	0.01529700	0.07996600
H	-11.69062100	1.62934200	0.85922800
H	-13.79124500	0.33096800	0.34898500
H	-13.00392900	-2.01497600	-0.74956000
H	-10.30412400	-1.97200300	-0.82628200
C	-4.25497700	-0.06666800	-0.16147800
C	-2.99633700	0.02085600	-0.11923800
C	-0.90611900	1.34335800	-0.03096700
C	0.54494300	1.38987100	0.03865800
C	1.29451400	0.15341200	0.07759600
C	0.60543200	-1.06859600	0.11581700
C	-0.82632400	-1.13587600	-0.00680700
C	-1.58630000	0.07491400	-0.06449900
C	-1.64648100	2.54222500	-0.08282600
C	-1.04197600	3.78809000	-0.08021500
C	0.39048700	3.84058800	-0.01576700
C	1.12450900	2.66575900	0.03433000
C	1.30210700	-2.25393700	0.32550700
C	0.68989500	-3.49806700	0.30712700
C	-0.73133000	-3.58190600	0.09487300
C	-1.44979400	-2.39788900	-0.03840500
H	-2.72165800	2.48851600	-0.12848200
H	2.19361400	2.79838600	0.07039900
H	2.36885000	-2.22307300	0.52982100
H	-2.52013000	-2.44857400	-0.15643400
C	9.09657600	-1.72830300	-0.23651400
N	9.72459500	-2.69878800	-0.32560100
C	1.02666000	5.12145300	-0.00872400
C	0.28857900	6.26031500	-0.06132800
C	-1.13467300	6.20625800	-0.12600500
C	-1.78079600	5.01232600	-0.13588400
C	-1.34604700	-4.87163500	0.04854000
C	-0.59939000	-5.99630700	0.20376700
C	0.80644800	-5.91246500	0.41918300
C	1.43216500	-4.70725500	0.47235800
H	2.10653200	5.17097500	0.03916700
H	0.78336000	7.22255700	-0.05498000
H	-1.70044800	7.12765000	-0.16792100
H	-2.86089800	4.97204200	-0.18628900
H	-2.41421100	-4.93887700	-0.11003100
H	-1.07343700	-6.96823800	0.16625500
H	1.37985800	-6.82200200	0.54041900
H	2.50040300	-4.65134100	0.63526500

P	9.35563500	0.94818900	0.05448800
O	10.81675500	0.75739500	-0.05974600
O	8.89422700	1.59965400	1.45383400
H	9.65701700	2.00636800	1.89926300
O	8.74125900	1.95231400	-1.04720600
H	9.45784100	2.41164300	-1.51729100

PPSQA3

C	6.37127200	0.26267400	0.59358400
C	5.53265200	1.44473300	0.59760600
C	4.39273400	0.66377300	0.02071400
C	5.29847200	-0.53461300	0.03224500
C	3.12178000	0.95872600	-0.34352800
H	2.79208400	1.98427600	-0.21533900
C	2.20669500	-0.02795800	-0.83434300
O	5.15335700	-1.71275200	-0.30676500
O	5.66099000	2.62671500	0.92937300
H	2.59158700	-1.04064900	-0.79282900
S	-6.61437500	-1.25346700	0.69593400
C	-8.00710500	-0.37946300	1.31063800
C	-7.76809200	0.98279400	1.33678500
C	-6.47954300	1.32528800	0.89036900
C	-5.69540900	0.25328900	0.50206700
N	-9.11806900	-1.08261000	1.67677200
H	-8.49002600	1.70551200	1.68403400
H	-6.11210100	2.34236000	0.85389300
H	-9.05263500	-2.09199400	1.68431900
N	-11.18072400	-1.27733700	2.85253700
C	-12.36205100	-0.59898900	3.04091100
C	-12.28244000	0.57832900	2.33775300
C	-11.01399600	0.61429600	1.68714600
C	-10.35896000	-0.55382200	2.02837200
H	-10.94595000	-2.16761700	3.26895800
H	-13.14496000	-1.01337800	3.65428700
H	-13.04935200	1.33568700	2.28330900
H	-10.64463700	1.38712600	1.03429800
C	-4.39387900	0.23827200	0.02697400
C	-3.24515300	0.21288500	-0.39352700
C	-1.31214800	-1.06004200	-1.22903000
C	0.10183700	-1.09546500	-1.50632500
C	0.90752400	0.11278500	-1.24962700
C	0.19682000	1.39516700	-1.35522600
C	-1.21583800	1.43365200	-1.06236100
C	-1.93343200	0.19306600	-0.84958400
C	-2.05535800	-2.23043900	-1.35336600
C	-1.48246500	-3.43903500	-1.78726900
C	-0.09050100	-3.45926500	-2.11675600
C	0.66139200	-2.27397300	-1.96134900
C	0.82676900	2.56529200	-1.73261000
C	0.16183000	3.81242700	-1.75436400
C	-1.21409100	3.86394500	-1.36957200
C	-1.86900500	2.66209800	-1.04338800
H	-3.11624300	-2.21205700	-1.13334300
H	1.71365100	-2.30700500	-2.21752800
H	1.86264800	2.54119000	-2.04296800
H	-2.92570100	2.69889500	-0.80660100
C	7.72398900	-0.01155100	0.99025000
C	8.27393300	-1.30594600	0.86662900
C	8.55037100	1.00493700	1.51681400
C	9.58049800	-1.56088600	1.25052300
H	7.65821700	-2.10199900	0.46584300

C	9.85483600	0.73321400	1.89611300
H	8.14951600	2.00592200	1.62137700
C	10.40904300	-0.55337500	1.77516500
H	9.97222800	-2.56639600	1.14196100
H	10.46267700	1.53705700	2.29694700
B	11.88006800	-0.85045300	2.20400900
C	0.81505400	5.01141700	-2.13562000
H	1.85793600	4.96792200	-2.43058600
C	-1.87995100	5.11935300	-1.36860700
C	-1.21658600	6.26356200	-1.73529900
H	-1.73389500	7.21606100	-1.73100900
C	0.14316800	6.20985300	-2.12496300
H	0.65318400	7.12137100	-2.41432000
H	-2.92362600	5.15748100	-1.07587500
C	0.48656100	-4.66741300	-2.58496700
C	-2.24051900	-4.63272100	-1.93228900
H	-3.29571600	-4.61488700	-1.68176500
C	-1.65039700	-5.78623300	-2.38382500
H	-2.23731200	-6.69118900	-2.49090000
C	-0.27360300	-5.80405000	-2.71458700
H	0.17868100	-6.72230300	-3.07099800
H	1.54181400	-4.67979700	-2.83566300
O	12.63605100	0.17849300	2.70962800
H	13.53870800	-0.06186700	2.95710500
O	12.36006300	-2.12889400	2.05844000
H	13.27650400	-2.25438800	2.33820500

PASQA1@TiO₂

C	-2.62106300	4.06441500	-0.30849800
C	-3.90354800	4.83019900	-0.44212700
C	-4.64968700	3.58304800	-0.40100000
C	-3.43040600	2.79196400	-0.29561600
C	-1.30754600	4.47816900	-0.28747300
C	-6.03213100	3.25624900	-0.45803800
H	-6.73134200	4.08875700	-0.49699900
C	-6.48069300	1.96539200	-0.42541000
O	-3.19111400	1.58439900	-0.25413300
O	-4.17054000	6.02820100	-0.53828000
H	-5.71336100	1.20313500	-0.32195600
S	-14.95556400	-2.07304600	0.64927500
C	-16.62134500	-1.85895300	0.11957600
C	-16.74124700	-0.77227400	-0.73302900
C	-15.51489100	-0.10797900	-0.95469600
C	-14.42918200	-0.65513500	-0.29323400
N	-17.58103800	-2.72730400	0.56641000
H	-17.68148100	-0.46297500	-1.16807600
H	-15.41703700	0.76780600	-1.58659500
H	-17.31368600	-3.42030200	1.25398500
N	-19.90009400	-3.18572200	0.94129500
C	-21.09539300	-3.22644500	0.25867500
C	-20.84572100	-2.85631400	-1.04506400
C	-19.44770000	-2.59345700	-1.16459700
C	-18.89233300	-2.80886300	0.08679000
H	-19.77983100	-3.38132400	1.92620300
H	-22.00724300	-3.51622300	0.75909600
H	-21.58008200	-2.78728600	-1.83626000
H	-18.91040400	-2.30720400	-2.05653600
C	-13.09381700	-0.24879500	-0.29813100
C	-11.92266500	0.10894900	-0.31871000
C	-9.57630300	-0.10508500	0.39167500
C	-8.21996400	0.37824500	0.36211700

C	-7.86224700	1.49926100	-0.45432100
C	-8.86211900	2.10337300	-1.27755700
C	-10.23056700	1.65212000	-1.21263500
C	-10.58132700	0.55167500	-0.37724900
C	-9.89847800	-1.22583800	1.21423000
C	-8.94693000	-1.84470900	1.98427500
C	-7.61494900	-1.35662500	1.98520100
C	-7.27012700	-0.27699200	1.21030900
C	-8.55437400	3.12130800	-2.23641000
C	-9.52543600	3.71204000	-3.00604400
C	-10.88196500	3.31764300	-2.87574900
C	-11.21595800	2.30534300	-2.01287500
H	-10.92270100	-1.58325000	1.22269800
H	-6.25356000	0.09262200	1.25859500
H	-7.52245500	3.41378100	-2.37733800
H	-12.24574300	1.97356300	-1.93559100
H	-9.21336400	-2.69734700	2.60185500
H	-6.86540600	-1.83358200	2.60992600
H	-9.25104400	4.47460300	-3.72908400
H	-11.64820600	3.79839600	-3.47674600
C	-1.00955300	5.86073200	-0.49505500
N	-0.73392000	6.98283200	-0.65689600
C	-0.14953600	3.59531200	-0.08013800
O	1.01430500	4.07493700	-0.35501000
O	-0.34574400	2.42130100	0.36626000
Ti	4.16252700	-3.86222500	-2.13643700
O	2.78429600	-2.59931900	-1.88582200
O	5.74619600	-4.36039600	-0.95228500
O	3.52452900	-5.53949700	-1.68349800
O	3.78126700	-1.96641600	1.18165000
O	5.99317100	0.71158100	-0.29984600
O	3.86887600	-0.34603000	-0.58801800
O	1.50673000	-2.94317300	0.64312900
O	7.72968600	-2.00607100	-2.25205300
O	5.38804200	-3.00767200	-3.33734600
Ti	7.67745600	-2.22876900	1.66933200
O	8.41319800	-3.49514900	0.33456600
O	6.46753100	-1.97020000	0.19553200
O	3.47570900	-4.76725200	1.56513000
O	1.87539300	-2.08459100	3.32140200
Ti	5.18103000	-0.66078500	0.90382800
Ti	5.82818200	0.49066700	3.63302000
O	6.46503400	-0.90049000	2.40313000
O	4.55297600	0.63526700	2.17717100
Ti	2.61309700	-3.14377900	1.97767300
Ti	7.22907800	-3.22149800	-0.93428300
Ti	4.31068500	-5.28904400	-0.01465100
O	4.82903400	-0.07357000	-3.21963700
O	1.09463800	-0.44401400	-0.50160700
Ti	4.60802500	0.95008000	-1.79043000
O	3.16877700	2.11519300	-1.73791100
Ti	2.47329800	-1.64752400	-0.41923000
Ti	6.23055700	-1.31823700	-3.47061500
O	7.60667500	-0.50729000	-4.39356100
O	5.87750700	2.35823600	-2.20351500
O	8.45862600	1.25572300	-1.69302400
O	6.58904700	3.43092800	0.35916000
Ti	7.00716500	2.10440400	-0.89731400
Ti	8.46507300	-0.27190000	-2.76407800
Ti	0.75129100	0.75590100	0.81824400
O	2.02258300	1.16270700	3.77254700
O	-0.28522800	0.06220500	2.17128300

O	4.02257400	3.68247600	2.31749100
O	2.28232100	1.92525400	1.05527300
O	4.66112500	1.82965000	4.32017600
Ti	3.48656300	1.95607000	2.97157600
Ti	1.14564400	-0.35948700	3.22608500
Ti	2.79240400	3.07644800	-0.25936800
Ti	4.97804600	4.17643100	0.88056100
H	3.12747200	5.75809000	-0.26631100
O	3.61983000	4.92338000	-0.33163000

PASQA2@TiO₂

C	-3.28116500	1.71659800	-1.87211400
C	-4.37709900	1.80192400	-2.90571100
C	-5.27789500	1.10370000	-2.00531600
C	-4.24001800	0.94552300	-0.99925800
C	-2.01014300	2.20509900	-1.79298600
C	-6.66281700	0.77558100	-2.05833200
H	-7.20458800	1.10044700	-2.94448700
C	-7.32566600	0.17351000	-1.02840300
O	-4.17837500	0.42472900	0.11881900
O	-4.44450800	2.30243100	-4.02772100
H	-6.73230900	-0.03900300	-0.14457000
S	-16.35624600	-0.18580900	1.30731100
C	-17.97788100	-0.40601700	0.65832800
C	-17.93970800	-0.76267500	-0.67952600
C	-16.62419800	-0.84094500	-1.19226500
C	-15.62714900	-0.55946500	-0.27641600
N	-19.05411500	-0.22027100	1.48369900
H	-18.82792700	-0.94157900	-1.26989600
H	-16.40061400	-1.09130000	-2.22335800
H	-18.88151300	0.14825600	2.41109200
N	-21.40339900	0.17637200	1.71717100
C	-22.61100300	-0.34938200	1.31429500
C	-22.34645400	-1.42941600	0.50097000
C	-20.92840200	-1.57568300	0.41570900
C	-20.37552400	-0.56215700	1.18223600
H	-21.28442700	0.99563600	2.29797000
H	-23.54095600	0.08869000	1.64458800
H	-23.08461100	-2.05909700	0.02278700
H	-20.38071000	-2.33811400	-0.11802000
C	-14.24089000	-0.52089900	-0.44299500
C	-13.02321200	-0.47401300	-0.56150800
C	-10.83471300	0.01677900	0.45143100
C	-9.40929200	0.17541200	0.31469800
C	-8.75959900	-0.08996000	-0.93536200
C	-9.53729900	-0.59088100	-2.02129300
C	-10.97114300	-0.70500900	-1.90132600
C	-11.61413000	-0.38679000	-0.67316400
C	-11.44713400	0.29549300	1.71098900
C	-10.71138900	0.72099000	2.78719700
C	-9.31122500	0.90949900	2.65403900
C	-8.68852700	0.65464000	1.45785300
C	-8.94444000	-1.05682800	-3.23773300
C	-9.70191400	-1.50867100	-4.28946000
C	-11.11778200	-1.53413800	-4.19334400
C	-11.72723300	-1.15703500	-3.02397000
H	-12.51977000	0.16513000	1.80462800
H	-7.62406700	0.83525200	1.38110400
H	-7.86536900	-1.08113400	-3.31720200
H	-12.80702000	-1.21112700	-2.92988200
C	-1.50539000	2.95680500	-2.88711500

N	-1.04240800	3.59128400	-3.75099200
P	-0.91260800	2.04410300	-0.32957800
O	0.38709000	2.81658800	-0.81060800
O	-0.53888200	0.50114300	-0.27415700
O	-1.51540200	2.60881400	0.92596900
Ti	6.24837000	-3.22669500	-2.21024200
O	4.46907500	-2.56048100	-2.28487500
O	7.80532600	-3.41658400	-0.82338000
O	6.04869500	-5.09129200	-1.75851700
O	4.68012000	-1.96834000	1.02266200
O	6.05384500	1.46171900	0.27461500
O	4.59260800	-0.23755700	-0.66975600
O	3.05874700	-3.60196800	0.00463100
O	9.09382300	-0.26637000	-1.54252700
O	7.21624900	-1.70786200	-2.79102900
Ti	8.24900500	-1.11203500	2.20220600
O	9.58872500	-1.84774800	0.95430400
O	7.32668100	-0.98545500	0.51703800
O	5.33223800	-4.66759300	1.35232000
O	2.61442900	-2.83265700	2.75009800
Ti	5.56471900	-0.27266700	1.09710700
Ti	5.24203700	0.56006800	3.96194500
O	6.58684300	-0.27780700	2.79145600
O	4.30482100	0.59020200	2.27840800
Ti	3.87378200	-3.53838500	1.53622000
Ti	8.64502000	-1.77213900	-0.51688800
Ti	6.53225500	-4.65943900	-0.08172100
O	5.92526400	0.86695100	-2.94427200
O	2.00206800	-1.26984500	-0.97499400
Ti	5.05545800	1.43763600	-1.51540100
O	3.31849800	2.01217100	-1.74273900
Ti	3.71395900	-1.93538300	-0.80596200
Ti	7.68749200	0.15315500	-2.96312100
O	8.82217200	1.67074400	-3.26015000
O	5.74395000	3.27991500	-1.43213000
O	8.33369400	2.98384000	-0.39726400
O	5.31397100	4.02486200	1.30300300
Ti	6.54999800	3.20759500	0.10250200
Ti	9.11512700	1.68461400	-1.48274700
Ti	1.06914500	-0.41738400	0.30973800
O	1.41817800	0.06236300	3.31034100
O	-0.11718900	-1.71121000	1.29987100
O	2.58020900	3.19009500	2.61394100
O	2.02054800	1.11565400	0.77865200
O	3.58777000	1.36800100	4.49493900
Ti	2.72000700	1.35241900	2.93330800
Ti	1.21524300	-1.65216100	2.74139100
Ti	2.25761700	2.55725500	-0.38801000
Ti	3.50680500	4.19489500	1.41549800
H	1.70250600	5.16736300	-0.35134100
O	2.41612300	4.53292000	-0.16643200
H	-1.09121800	-1.66666800	1.27148200
H	-8.72982300	1.26603200	3.50097500
H	-11.19991600	0.92366800	3.73732100
H	-9.21493600	-1.86500100	-5.19408100
H	-11.71367700	-1.87995800	-5.03468900

PASQA3@TiO₂

C	-5.68923800	-1.14580900	-0.48893800
C	-6.66411600	-2.22913700	-0.74574700
C	-7.79060800	-1.33279300	-0.36493500

C	-6.80567500	-0.24089500	-0.15317300
C	-9.16250400	-1.46144100	-0.23279400
H	-9.58614200	-2.44134100	-0.44583800
C	-10.01226900	-0.39331500	0.12083600
O	-6.89316600	0.96482300	0.21216400
O	-6.57699600	-3.43757100	-1.09377600
H	-9.50956200	0.56790500	0.13025000
S	-18.98126000	1.61519200	-0.67644900
C	-20.66820600	0.91559000	-0.75978700
C	-20.64595300	-0.44656100	-0.55395100
C	-19.34220700	-0.98751600	-0.34123400
C	-18.29876800	-0.08513800	-0.36849100
N	-21.72237100	1.77540200	-0.98487500
H	-21.53918400	-1.05588900	-0.56737600
H	-19.17031900	-2.04452500	-0.17192700
H	-21.51135900	2.72629500	-1.26174600
N	-24.02597900	2.13228100	-1.58605600
C	-25.29611500	1.67281500	-1.25853000
C	-25.14616700	0.68182300	-0.30583000
C	-23.74551300	0.53783800	-0.03050600
C	-23.07765700	1.45211700	-0.83956000
H	-23.82008600	2.83978600	-2.27749800
H	-26.17501100	2.08881300	-1.72386500
H	-25.94465100	0.12078700	0.15787400
H	-23.29240300	-0.13016100	0.68458200
C	-16.92483400	-0.25736300	-0.20287500
C	-15.70770300	-0.36576600	-0.04154400
C	-13.58198200	0.87588100	0.15251700
C	-12.14720300	0.88157400	0.28654000
C	-11.40900200	-0.38251500	0.35682100
C	-12.18962900	-1.57667600	0.65884300
C	-13.62280200	-1.57584600	0.49488500
C	-14.31262500	-0.36286500	0.16598200
C	-14.26315800	2.12358100	0.00946500
C	-13.58830600	3.32773900	0.02240200
C	-12.18309700	3.34206600	0.18358800
C	-11.49228700	2.14834100	0.30337900
C	-11.59143500	-2.75433100	1.19646600
C	-12.31676600	-3.90859900	1.44221000
C	-13.70289400	-3.93707400	1.16130500
C	-14.33687600	-2.79349500	0.71616800
H	-15.34266300	2.11118100	-0.09887500
H	-10.41871100	2.19609600	0.43451100
H	-10.54375500	-2.73160200	1.46424300
H	-15.41006300	-2.79755000	0.55735800
C	-4.29859000	-1.00145300	-0.52461600
C	-3.68676100	0.25880800	-0.18941300
C	-3.41282900	-2.09012100	-0.85290100
C	-2.32042500	0.40404200	-0.15290800
H	-4.33610700	1.09438600	0.05084700
C	-2.04494900	-1.93952600	-0.80530100
H	-3.85149000	-3.04785800	-1.11463300
C	-1.44772600	-0.69289700	-0.44008300
H	-1.88347300	1.35770000	0.12103900
H	-1.39833300	-2.78076500	-1.03566900
C	-0.04661300	-0.54884800	-0.30483400
O	0.77367300	-1.53126600	-0.65039200
O	0.45666000	0.56484000	0.22079100
Ti	8.41009200	-0.37041700	-3.47751900
O	6.55783600	-0.69337800	-3.16959700
O	9.77724000	-0.47675800	-1.97977300
O	9.28565500	-1.85533600	-4.22009700

O	6.79069900	-1.76946300	-0.12596700
O	6.31498700	1.84054200	0.96456200
O	5.58052800	0.22836200	-0.67317900
O	5.97140600	-3.24490000	-2.02491500
O	9.35357000	2.58883900	-1.04542400
O	8.62217600	1.52883400	-3.52074700
Ti	9.69263200	-0.06254400	1.97624000
O	11.09098800	0.58588700	0.70277000
O	8.61978400	0.34698800	0.38773400
O	8.66428900	-3.51694400	-1.33097800
O	5.61469200	-4.27251300	0.60212200
Ti	6.79891700	-0.09547400	0.92216700
Ti	6.46960100	-0.90462100	3.87366200
O	7.88304200	-0.49812900	2.58355800
O	5.43739900	-0.62757800	2.22516400
Ti	6.94297000	-3.56994000	-0.57985400
Ti	10.03142200	0.88018000	-0.72185800
Ti	9.67357800	-2.38031800	-2.44420700
O	6.11547400	2.58087000	-2.16702400
O	3.77739600	-1.54808000	-1.83638600
Ti	5.15601300	2.09946900	-0.73481700
O	3.31069900	1.81796200	-0.79962000
Ti	5.63005300	-1.33649800	-1.78073600
Ti	7.95352700	2.96839800	-2.45969300
O	8.37640500	4.78408900	-2.19606700
O	4.98868300	3.83682000	0.12678900
O	7.57483400	4.41689900	1.07604400
O	4.63163700	3.19373400	2.87448700
Ti	5.98004500	3.55989100	1.57742000
Ti	8.74839200	4.34284100	-0.40259500
Ti	2.70763800	-1.94999100	-0.41832100
O	3.41858100	-2.90176500	2.44047400
O	2.30160000	-3.88965100	-0.23152400
O	2.92801600	0.55518900	3.43216800
O	2.91520800	-0.63046700	0.91469500
O	4.68908300	-1.39124400	4.46259000
Ti	3.75596800	-1.09209100	2.93089100
Ti	3.82908600	-3.98904100	1.04266000
Ti	2.32896400	1.13842300	0.58008200
Ti	3.01112300	2.30018700	2.95177800
H	0.53441100	2.73634200	1.80912000
O	1.49103600	2.56873900	1.69820900
H	1.47834400	-4.39636800	-0.36007900
H	-14.13471100	4.25988200	-0.08105700
H	-11.64747200	4.28504500	0.21584300
H	-14.27497900	-4.84296200	1.33615500
H	-11.82811900	-4.77849700	1.86824100

PPSQA1@TiO₂

C	2.29693300	-4.07000800	-0.47865800
C	3.52762600	-4.89332200	-0.46967600
C	4.30881700	-3.73829800	-0.92248300
C	3.08044000	-2.92832700	-1.01046900
C	0.99421500	-4.36966400	-0.05973500
C	5.66986200	-3.48257100	-1.11006100
H	6.35439900	-4.29972600	-0.90389900
C	6.12635000	-2.21437900	-1.46346200
O	2.84084200	-1.78834100	-1.41994000
O	3.77646000	-6.06690000	-0.18249400
H	5.32628200	-1.48661700	-1.54407900
S	13.52079800	2.80450400	0.67769300

C	15.17408900	2.68471700	1.26966400
C	15.62888400	1.37529000	1.22725800
C	14.65894200	0.46899400	0.74949100
C	13.44555300	1.04305000	0.40487200
N	15.81137500	3.82135100	1.68621400
H	16.61696300	1.08262600	1.55359500
H	14.83025900	-0.59817000	0.66459000
H	15.26355900	4.66998800	1.76229800
N	17.58794900	4.86538600	2.89701100
C	18.96145000	4.84207500	2.99392700
C	19.42582600	3.87989300	2.12413400
C	18.29826100	3.30487000	1.46457300
C	17.17483100	3.94204300	1.96820200
H	16.97018500	5.45200700	3.44229800
H	19.47829400	5.50992900	3.66649000
H	20.46285100	3.61791400	1.96417900
H	18.30712500	2.54524500	0.69767100
C	12.28234800	0.44932900	-0.07379200
C	11.23351300	-0.02814300	-0.49665000
C	8.92222400	0.30365700	-1.26244100
C	7.62968200	-0.26245800	-1.60323900
C	7.44272500	-1.70696800	-1.58444300
C	8.62861600	-2.53846600	-1.59219800
C	9.91608200	-1.97450800	-1.22840600
C	10.03181900	-0.56292700	-0.98078200
C	9.07171600	1.70002900	-1.20371800
C	8.02559400	2.57826400	-1.49448700
C	6.74842000	2.02485900	-1.87015100
C	6.59206000	0.63344900	-1.90782600
C	8.59232100	-3.89008800	-1.96188200
C	9.71679900	-4.72605100	-1.90901700
C	10.97286600	-4.18116900	-1.45864000
C	11.03593300	-2.82027800	-1.14509300
H	10.04127000	2.11228000	-0.94137200
H	5.62127000	0.26043800	-2.21233100
H	7.67374200	-4.31449100	-2.34796200
H	11.99239500	-2.39601700	-0.85858700
C	0.69710900	-5.71881200	0.29885900
N	0.42165000	-6.81184100	0.59760000
C	-0.08597200	-3.42250300	0.10493500
O	-1.24246200	-3.88655400	0.46976800
O	0.12135000	-2.16895100	-0.06619300
C	5.68015400	2.91897400	-2.19270900
C	5.86162500	4.27735000	-2.13782200
C	7.12475900	4.82484600	-1.76096200
C	8.17530000	4.00076800	-1.45028800
C	12.11259900	-5.04263400	-1.38739800
C	12.01505000	-6.36224100	-1.74767100
C	10.77486100	-6.89813500	-2.20594400
C	9.65995400	-6.10254900	-2.28729800
H	4.71916700	2.49915900	-2.47887100
H	5.04208800	4.94714000	-2.38156800
H	7.24787800	5.90337400	-1.72346100
H	9.13949400	4.41360600	-1.16557100
H	13.05704700	-4.62904300	-1.04376800
H	12.88555200	-7.00910400	-1.68875400
H	10.71839900	-7.94510200	-2.48937000
H	8.71325500	-6.50998200	-2.63226400
Ti	-5.92981500	2.23869200	-3.26630200
O	-4.41185500	1.17731400	-2.96940300
O	-7.00658400	3.34394800	-1.91002700
O	-5.45273700	3.87238200	-3.99067300

O	-4.13366800	2.19041800	0.11183500
O	-6.35248700	-0.72367100	1.03501600
O	-4.61070900	-0.08985600	-0.47395800
O	-2.37508600	2.63337100	-1.65697300
O	-8.92999000	0.83295700	-1.14929300
O	-7.39081900	1.05362000	-3.47324000
Ti	-7.52749900	2.92739500	1.93074100
O	-8.87483800	3.44503000	0.57940000
O	-6.94586800	1.91708600	0.40393300
O	-4.12085500	4.78832300	-1.08096500
O	-1.65406900	3.30367700	1.00941300
Ti	-5.35149500	0.97974200	1.03385100
Ti	-4.72423800	1.33395800	3.99345600
O	-5.94567200	2.04132300	2.63695900
O	-4.09473400	0.44174100	2.38573900
Ti	-2.96025300	3.55281600	-0.28754900
Ti	-8.24357500	2.52690400	-0.78842200
Ti	-5.52160700	4.55582900	-2.27096100
O	-6.41378000	-1.46596900	-2.11909400
O	-2.01192000	-0.11127500	-1.52499200
Ti	-5.57822000	-1.74123000	-0.59197800
O	-4.07738300	-2.80709100	-0.61694700
Ti	-3.43507500	1.04121200	-1.49394200
Ti	-7.96359000	-0.42237200	-2.42620200
O	-9.43872300	-1.50671500	-2.27293100
O	-6.71266800	-3.08903800	0.21853100
O	-9.01133100	-1.70487700	1.04071000
O	-6.14854600	-2.72013700	2.99382900
Ti	-7.29639800	-2.18009800	1.58681700
Ti	-9.60339900	-0.88210700	-0.51263000
Ti	-0.99655300	-0.48304700	-0.06925500
O	-1.11015500	0.64376000	2.91825100
O	0.26987500	0.79483500	0.30364400
O	-3.09006200	-2.15880900	3.68760600
O	-2.21067200	-1.32138300	1.19297600
O	-3.22803600	0.42147100	4.67733600
Ti	-2.61031600	-0.37317400	3.17941900
Ti	-0.74754700	1.73121800	1.47497800
Ti	-2.97099600	-2.93959600	0.80744000
Ti	-4.39316800	-3.25459700	3.11504200
H	-2.86719100	-5.26600400	2.12656200
O	-3.47193300	-4.53138500	1.91907000

PPSQA2@TiO₂

C	2.13347900	3.66134700	1.53903300
C	3.41870000	3.93342300	2.27963300
C	4.05662000	2.82657000	1.58229500
C	2.84234800	2.50719700	0.86589200
C	0.90977900	4.26750300	1.50159400
C	5.38216800	2.30460900	1.58492900
H	6.06233800	2.73331400	2.31984800
C	5.83807500	1.35710000	0.71604300
O	2.55310100	1.63406300	0.02675800
O	3.74718200	4.76509500	3.12285500
H	5.13950800	1.00932900	-0.04024600
S	14.67325900	-1.01822700	-1.42805600
C	16.22744800	-1.34628100	-0.67193700
C	16.11255100	-1.40648500	0.70840200
C	14.79784000	-1.15702900	1.16172100
C	13.87210100	-0.92079400	0.15886500
N	17.32942200	-1.49661200	-1.46954500

H	16.95195000	-1.59493900	1.36387800
H	14.52080400	-1.14309700	2.20991400
H	17.21950800	-1.34105900	-2.46452200
N	19.71533100	-1.44921000	-1.66122500
C	20.83252000	-2.03320000	-1.10794000
C	20.40931500	-2.88401700	-0.10941800
C	18.98404500	-2.82731500	-0.06250700
C	18.58757200	-1.93161400	-1.04249300
H	19.71929500	-0.75369700	-2.39543300
H	21.81966700	-1.79389300	-1.47400600
H	21.04665600	-3.49272200	0.51762100
H	18.32804500	-3.39193300	0.58361500
C	12.50957800	-0.63801300	0.25597300
C	11.31542300	-0.37147300	0.32883900
C	9.19289400	0.24532100	-0.74888800
C	7.81251800	0.68492800	-0.63570700
C	7.19786900	0.83006100	0.64871800
C	7.93169500	0.45957700	1.81885500
C	9.32588000	0.05314500	1.71509300
C	9.95136500	-0.02628300	0.43178200
C	9.77199600	0.12240500	-2.02849300
C	9.07037300	0.41352000	-3.19537800
C	7.70358500	0.87700100	-3.08998300
C	7.12542600	1.00876500	-1.82949200
C	7.33381000	0.42612400	3.10092700
C	8.03947300	0.08936700	4.25304500
C	9.44291300	-0.24873600	4.14912000
C	10.03677500	-0.26572200	2.89068100
H	10.80209100	-0.21028000	-2.10740200
H	6.10997700	1.38382000	-1.77812600
H	6.27918800	0.65337300	3.19792300
H	11.08098000	-0.54992400	2.80895400
C	0.63420900	5.41206200	2.29091400
N	0.29809100	6.34162300	2.91487900
C	6.99087900	1.19511700	-4.29386700
C	7.58786500	1.05847600	-5.51722300
C	8.93897400	0.59593100	-5.62069300
C	9.65619400	0.28427200	-4.49795300
C	10.16205400	-0.58197900	5.34453200
C	9.53231500	-0.58929900	6.55907300
C	8.14109100	-0.26548100	6.66149300
C	7.41876300	0.06059600	5.54655000
H	5.96497700	1.54441200	-4.21106200
H	7.03904800	1.30010100	-6.42279300
H	9.39148400	0.49541400	-6.60298900
H	10.68230800	-0.06603200	-4.57227500
H	11.21689500	-0.83091200	5.26338300
H	10.08506000	-0.84341500	7.45891600
H	7.66336500	-0.27996900	7.63683200
H	6.36359600	0.30998600	5.62102900
P	-0.35620800	3.64800600	0.33979200
O	-1.77488200	4.19975800	0.80411900
O	-0.34929100	2.11190400	0.70447600
O	-0.01384900	4.00841100	-1.08060500
Ti	-5.22995000	-3.87116000	2.14617600
O	-3.79345800	-2.62473300	2.35606300
O	-6.53326400	-4.54273100	0.76097000
O	-4.24081100	-5.43409800	1.48511900
O	-3.98869600	-2.02903000	-0.96201300
O	-6.49788600	0.69331700	-0.25702600
O	-4.58509500	-0.39937800	0.71625800
O	-1.94198400	-2.99666200	0.15537900

O	-8.78348700	-1.77446100	1.41832800
O	-6.63343700	-2.69573300	2.62053500
Ti	-7.63871700	-2.53093100	-2.18242300
O	-8.71217100	-3.59355700	-0.91790600
O	-6.81300400	-2.07479200	-0.50087400
O	-3.56513200	-4.70243000	-1.43883000
O	-1.57885600	-2.08603400	-2.59950000
Ti	-5.42599600	-0.78327100	-1.06018500
Ti	-5.39354300	0.04483100	-3.95383100
O	-6.28002800	-1.24840700	-2.77454300
O	-4.61096500	0.49884700	-2.24853400
Ti	-2.60143500	-3.14528500	-1.45771800
Ti	-7.84795000	-3.19215600	0.55665800
Ti	-4.87016300	-5.09800300	-0.12799400
O	-6.18665800	0.20758200	2.94826600
O	-1.89838500	-0.46846000	1.22513200
Ti	-5.57142400	1.05469200	1.52435900
O	-4.16320200	2.23581400	1.77505700
Ti	-3.21799500	-1.73855600	0.93891300
Ti	-7.63019300	-1.02661100	2.87127900
O	-9.17937500	-0.05747200	3.30868800
O	-6.89827800	2.48790200	1.45233500
O	-9.24164000	1.33481800	0.31220000
O	-6.89300100	3.38805400	-1.27219900
Ti	-7.61698500	2.11891700	-0.08870900
Ti	-9.58045400	-0.04780300	1.52425700
Ti	-1.39910700	0.70220400	-0.05929100
O	-1.66648300	1.02420200	-3.17438300
O	0.28055100	0.16958300	-0.94563800
O	-4.01110000	3.50690400	-2.57079300
O	-2.74394500	1.85557500	-0.69155200
O	-4.11561800	1.39980200	-4.46450300
Ti	-3.37432300	1.75611000	-2.87889800
Ti	-0.82910600	-0.41211900	-2.45923300
Ti	-3.42480000	3.17682200	0.42711600
Ti	-5.23331200	4.13380900	-1.38692400
H	-3.85630400	5.80486100	0.23668800
O	-4.31493200	4.95035000	0.16022200
H	1.07437200	0.70927600	-0.70773000

PPSQA3@TiO₂

C	-5.05757200	0.83038100	-0.44090100
C	-5.98613900	1.95284200	-0.26693800
C	-7.13990100	1.07670100	-0.65485400
C	-6.16439400	-0.05078100	-0.82080400
C	-8.48580300	1.24839700	-0.80684200
H	-8.88791500	2.23811800	-0.60600100
C	-9.36004300	0.18159700	-1.17707400
O	-6.27315900	-1.23693800	-1.14930400
O	-5.88251900	3.13827900	0.05522400
H	-8.87098200	-0.78748400	-1.21866200
S	-17.98423800	-1.59137000	1.47960800
C	-19.30492900	-0.70905100	2.25118600
C	-19.07497500	0.64697900	2.23168100
C	-17.83835500	0.99589900	1.61961800
C	-17.09987800	-0.07303100	1.15474700
N	-20.36858700	-1.42589800	2.75807800
H	-19.75702800	1.37097200	2.65743500
H	-17.48911800	2.01830500	1.52647100
H	-20.29514600	-2.43452100	2.77630600
N	-22.29501500	-1.57533900	4.16291800

C	-23.44644400	-0.87673500	4.46396600
C	-23.43282200	0.28423400	3.72576300
C	-22.24204000	0.28885100	2.93562400
C	-21.56013000	-0.88153000	3.23180200
H	-22.02047400	-2.45760600	4.57329200
H	-24.16074000	-1.26971300	5.17161000
H	-24.19537900	1.05153800	3.73675700
H	-21.93581500	1.03942700	2.22267700
C	-15.85502000	-0.11076300	0.51578500
C	-14.76082100	-0.11587400	-0.04031400
C	-12.81590100	-1.19167200	-1.12619100
C	-11.44042100	-1.08625200	-1.58191100
C	-10.72593400	0.19243200	-1.39965800
C	-11.56528700	1.39608000	-1.37024000
C	-12.93354800	1.28307400	-0.89946800
C	-13.49662500	-0.01323800	-0.64310000
C	-13.43433100	-2.45085200	-1.19829000
C	-12.79685800	-3.58237300	-1.73201500
C	-11.45549800	-3.45663800	-2.23827100
C	-10.82105300	-2.19909800	-2.14109000
C	-11.09423400	2.63533300	-1.78570900
C	-11.85890900	3.81849300	-1.68000500
C	-13.17896400	3.72628200	-1.11656100
C	-13.67813900	2.46395700	-0.75503200
H	-14.45843000	-2.55220400	-0.85124500
H	-9.81116300	-2.11065800	-2.53040700
H	-10.10742200	2.70942800	-2.22918900
H	-14.69791400	2.39700300	-0.38474100
C	-3.66067600	0.65748200	-0.31005700
C	-3.05039000	-0.61009800	-0.55317800
C	-2.80467000	1.74106500	0.05302200
C	-1.68616100	-0.77575100	-0.45144100
H	-3.68998600	-1.44189600	-0.83008600
C	-1.43963800	1.57213900	0.14848800
H	-3.25561800	2.70942200	0.24454800
C	-0.83387000	0.31057300	-0.10652700
H	-1.24440600	-1.74557000	-0.64786200
H	-0.81029200	2.41304600	0.41653500
C	0.63009200	0.12940700	-0.04199800
C	-11.36783200	5.08461000	-2.10044800
H	-10.36938700	5.13957500	-2.52840100
C	-13.94314300	4.92640200	-0.98853600
C	-13.43368200	6.13625700	-1.39840500
H	-14.03017200	7.03859100	-1.29321300
C	-12.13245500	6.22167800	-1.96348800
H	-11.74592700	7.18472900	-2.28392600
H	-14.94173500	4.86489900	-0.56255700
C	-10.81948200	-4.59235900	-2.81174400
C	-13.43515500	-4.85748200	-1.82068300
H	-14.44874800	-4.95997900	-1.44014800
C	-12.78837500	-5.93549800	-2.37734800
H	-13.29076300	-6.89748900	-2.43592400
C	-11.46538900	-5.80658100	-2.88093900
H	-10.96911700	-6.66806300	-3.31828500
H	-9.80631700	-4.48395600	-3.19217800
O	1.41898900	1.14809900	0.25646800
O	1.16332600	-1.05018100	-0.28318300
Ti	8.58171200	1.32453800	3.42288400
O	6.72054200	1.34137100	3.13290400
O	10.03020200	1.26931200	2.11006000
O	9.19322400	3.01774400	3.78444500
O	7.23962000	1.81319200	-0.04986700

O	7.07592700	-1.92313100	-0.27673000
O	6.11874700	-0.05906900	0.74724400
O	6.15286600	3.57527600	1.35242800
O	9.87137900	-1.93669200	1.92573500
O	9.01598700	-0.40689100	4.08314200
Ti	10.43247500	-0.20819400	-1.44659100
O	11.71841900	-0.23000900	-0.04082200
O	9.23811200	-0.16507400	0.06607800
O	8.88383700	4.08129100	0.63440200
O	6.18261400	4.05394300	-1.49381400
Ti	7.46255600	-0.03219500	-0.75139100
Ti	7.36115900	0.03788200	-3.79697200
O	8.67950000	0.04308000	-2.31210600
O	6.24841900	0.08092900	-2.20623200
Ti	7.25157000	3.62359200	-0.01961900
Ti	10.59545000	-0.32629000	1.29315100
Ti	9.80865000	3.20996500	2.06767200
O	6.56190500	-1.79035300	2.93040400
O	4.11197800	1.69587600	1.55412400
Ti	5.80910100	-1.88275600	1.33360700
O	3.94122000	-1.67459700	1.32085800
Ti	5.98949100	1.69756700	1.56510900
Ti	8.41313700	-1.99339800	3.22634100
O	8.84252200	-3.77424900	3.39170700
O	5.79213900	-3.72458200	0.88051200
O	8.45942900	-4.41543900	0.12526700
O	5.80730700	-3.86001800	-2.00027900
Ti	6.90167500	-3.71559400	-0.48272000
Ti	9.45386200	-3.82430200	1.65346400
Ti	3.29250500	1.70787400	-0.01522200
O	4.10638900	2.05563000	-3.13386700
O	2.99986000	3.60016100	-0.68495600
O	3.91560600	-1.48492900	-3.36928600
O	3.75464500	0.17722600	-1.01932600
O	5.68175400	0.32124800	-4.54779700
Ti	4.63366400	0.23675600	-3.08701000
Ti	4.53432900	3.25673200	-1.88648400
Ti	3.14488400	-1.40044700	-0.24092300
Ti	4.26248000	-2.86330500	-2.27836900
H	1.76601100	-3.15490100	-1.55159500
O	2.66274500	-3.15081100	-1.16065400
H	2.03215300	3.80373900	-0.68628600